

International scientific meeting

Breath Analysis in Physiology and Medicine



4th and 5th September 2006 Prague. Czech Republic.

About 90 participants will meet to discuss and exchange ideas in a series of specialized workshops.

Organised by

J. Heyrovsky Institute of Physical Chemistry,
Academy of Sciences of the Czech Republic
In collaboration with the
"International Association for Breath Research", IABR.

Venue:

J. Heyrovsky Institute of Physical Chemistry,
Dolejskova 3
Praha 8
Prague, Czech Republic

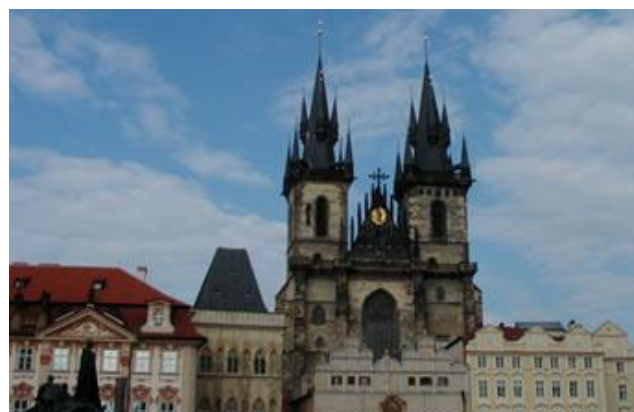


International organising committee

Anton Amann
Lars Gustafsson
Gennadiy V. Kamarchuk
Junichi Koizumi
Terence H. Risby
Giovanni Rolla
Mel Rosenberg
Jochen Schubert
David Smith
Patrik Španěl

Local organising committee

Patrik Španěl
Jiří Kubišta
Kseniya Dryahina
Ján Žabka
Ondřej Votava
Milan Mašat



International scientific meeting
Breath Analysis in Physiology and Medicine

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J. Heyrovsky Institute of Physical Chemistry, Dolejskova 3, Praha 8, Prague, Czech Republic

PROGRAMME

Monday 4th September

8:15 Registration, display of posters. Upload of the presentation files.

8:55: Introductory remarks

9:00 Workshop 1. New techniques in breath analysis (Anton Amann, 13 contributions, 120 min)

11:00 Coffee break

11:30 Workshop 2. Methodology (Joachim Pleil, 9 contributions, 90 min)

13:00 Lunch

14:00 Workshop 3. Breath markers in physiology (Terence Risby, 7 contributions, 90 min)

15:30 Coffee break

16:00 Workshop 6. Confounding variables in breath analysis (Claire Turner, 5 contributions, 90 min)

17:30 Poster session (32 posters)

18:45 End of poster session.

19:30: Cocktail Reception* at the Austrian Cultural Forum, Praha 1 - Jungmannovo náměstí 18.

Tuesday 5th September

8:30 Posters continued.

9:30 Workshop 4. Clinical breath analysis and lung function (Jochen Schubert, 7 contributions, 90 min)

11:00 Coffee break

11:30 Workshop 5. Metabolic disorders (Dietmar Fuchs, 8 contributions, 90 min)

13:00 Lunch

14:00 Workshop 7. In-vitro and urine studies (David Smith, 6 contributions, 90 min)

15:00 Coffee break

15:30 Panel discussion

17:30 End

* By invitation only. All conference participants will receive a separate invitation letter from Mr. Marco Freek. An invitation is just valid for one person and has to be presented at the entrance.
Created on 30/08/2006

Workshop 1. New techniques in breath analysis (13 contributions) 120 minutes

Name	FirstName	Summary
Amann	Anton	Workshop leader
Smith	David	An update of the developments made in SIFT-MS since the last meeting in Innsbruck will be presented, including the downsizing of the instrumentation for use in the clinical environment, improvements in sensitivity and in sampling methodology.
Baumbach	Jörg Ingo	Ion mobility spectrometry for metabolic profiling with respect to translational and personalized medicine: cell level, human organism and results of clinical studies. Personalized or translational medicine needs early information about changes in the inter- and extracellular noise. Metabolic profiling could contribute in addition to genomic and proteomic tools to find pre-dispositions, prognostic, diagnostic and therapeutic marker. Metabolomics includes also nutrition and environmental influence as well as interactions with pharmaceuticals. To realise an earlier response to changes in the cellular noise and to provide sufficient information in time to desire healthy and illness it's essential to bring a possibility of a decision also for future events if possible near to the presence. Sometimes, the gap between the first noisy change and the cancer detection takes more than two decades. The possibilities, advantages and disadvantages of ion mobility spectrometry for diagnostics and therapeutics will be considered in addition to genomic and proteomic tools. Inter- and extracellular noise and metabolites found in human breath will be included. To differentiate the grade of colon cancer on cell level results of investigations using IMS will be discussed. Metabolites of bacteria and molds are identified on cell level and in human breath. Considering Sarcoidose marker for patients showing clinical symptoms will be identified and clear decisions in the hospital supported directly. The effect of pharmaceuticals will be represented by metabolites in human breath, especially as function of time. It will be shown how IMS could support diagnostic and therapeutic decisions in a hospital within time intervals less than 10 minutes. Examples from interstitial lung diseases and Sarcoidose, chronic obstructive pulmonary disease (COPD), bronchitides, Pneumonia and bronchial carcinoma will be shown and discussed. Statistical and bioinformatic tools will be included in the discussion. Finally, IMS will be considered with respect to metabolomics. The need for platforms and databases should be noted, especially together with LC- and GC-MS and NMR investigations.
Thomas	Paul	Differential mobility spectrometry is a development in ion mobility spectrometry that provides significantly higher dimensionality data. The development of DMS methodologies for breath profiling provides sensitive and fieldable systems for breath profiling, and condition monitoring.
Alexy	Marcin	GE uses the advantages of Ion Mobility Spectrometry in security (e.g. airports, border crossings, prisons, customs) and sensing (e.g. cleaning validation) applications. The GE Security systems: EntryScan (walk-through portal), Itemiser (desktop detector) and VaporTracer (handheld) are successfully used to detect narcotics and explosives. Moreover, GE Sensing offers its Kaye Validator ITMS as fast, reliable and portable alternative to standard techniques for cleaning validation purposes in pharmaceutical industry. During the last few months GE researches from the European Global Research Center in Munich are looking into the opportunity to extend the ITMS portfolio of the company to breath analyzers for the healthcare business.
Mechold	Lars	This contribution focuses on the absorption spectroscopy using tunable diode lasers. An overview on tunable diode lasers and the basics of the method will be given. Some applications will underline its chances for breath analyzing due to the main advantages as selectivity, sensitivity and time response. Molecules of interest are C ₂ H ₆ , CH ₄ , CO, CO ₂ , C ₂ H ₄ and NH ₃ as well as isotopic species as ¹² CO ₂ and ¹³ CO ₂ .
Fritsch	Thomas	Laserspectroscopic Online Analysis of Exhaled Carbon Monoxide. For online monitoring of carbon monoxide in exhaled breath, a technique combining high sensitivity with good time resolution is needed. Our cavity leak-out spectrometer, based on a high-finesse cavity and a CO laser, achieves a detection limit of 7 ppb CO in breath (1 s integration time).
Kamarchuk	Gennadiy V.	Point-contact sensors for breath analysis: new prospects for a nanoscale sensitive technique in medicine. The new concept for the application of point contacts to gas sensors has been proposed and tested successfully. Point contacts have been used for human breath analysis and revealed both high sensitivity and selectivity to gas media under investigation. Point contact sensors appear to be promising tools for medical applications.
Pospelov	Olexandr P.	New active type sensors for breath gas analysis. New active type TCNQ derivatives-based sensors have been developed and applied successfully to breath gas analysis. High sensitivity and selectivity of new sensors were achieved by application of point-contact mesoscopic multistructures to sensor design. Characteristic parameters in sensor response to breath action were proposed to reveal correlations with organism state.
Ueda	Hideo	Compact gas chromatographic analyzers with a semiconductor detector and application to breath and biological specimen. Compact gas chromatographic analyzers with a semiconductor gas detector (GC/SCD) for breath and biological specimen were developed, and applied for clinical research. They are two kinds of analyzers, which measures simultaneously three (3) components of carbon monoxide (CO), methane (CH ₄) and hydrogen (H ₂), and four (4) components of acetone, isoprene, ethylalcohol and acetaldehyde, respectively. For CO/CH ₄ /H ₂ Analyzer, sample volume is 1.0ml and measuring time is four minutes. Detection limit is 0.1ppm, and is able to measure up to 100ppm, respectively
Donnay	Albert H	Sensitivity and suitability of encoded photometric infrared spectroscopy technology manufactured by Aspectrics.com for fast detection of multi-gas patterns involving both light gases (NO, CO, etc) and volatile organic chemicals in exhaled breath compared to ambient air.
Votava	Ondrej	Development and testing of high sensitivity absolute measurement technique for ammonia and other trace gasses in breath based on high resolution molecular spectroscopy in the near infrared spectral region will be presented. This method promises to be highly reliable and species specific and may lead to development of compact and affordable instrumentation for breath analysis.
Dweik	Raed	Recognition of Lung Cancer through Multidimensional Analysis of Exhaled Breath by an Electronic Nose. Electronic noses have been utilized in a variety of industrial applications. We used the electronic nose to evaluate exhaled breath samples from patients with lung cancer and those from other non-cancer groups. The electronic nose had 83.3 % and 87.5% specificity for detecting lung cancer. The positive and negative predictive values were 66.6 % and 94.5%, respectively. Thus, exhaled breath of lung cancer patients has distinct characteristics that can be identified with an electronic nose.

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Workshop 2. Methodology (9 contributions) 90 minutes

Name	FirstName	Summary
Pleil	Joachim D.	Workshop leader. The U.S. Environmental Protection Agency is developing risk assessment guidance for the exposure to diesel exhaust. Subjects are exposed under controlled conditions in an environmental chamber under a prescribed activity regimen. Blood, breath, and urine samples will be analyzed to assess the pre-clinical effects of the exposures. The focus of this work is the expression of endogenous organic compounds in exhaled breath condensate.
Sawano	Makoto	New techniques in breath analysis. We developed new technique of measuring carboxyhaemoglobin fraction (COHb%) by breath analysis. The technique consists of calculation of end tidal CO (ETCO) from expired CO and CO ₂ , and conversion of ETCO to COHb% by Haldane's equation. The technique enables real-time, non-invasive, continuous measurement of COHb% with 5-times high-resolution of CO-haemoximetry.
Basanta	Maria	An adaptive sampler for use with subjects with impaired respiratory function has been developed and it has been used to selectively sample different parts of the breathing profile in COPD subjects over a period of 10 to 15 minutes. GC-MS and GC-differential mobility spectrometry approaches are described.
Nose	Kazutoshi	Chemical compounds released from the skin are not well known, possibly because appropriate sampling methods to detect the low levels of the skin gas have not been established. In the present study, we developed a new gas-trap system for the analysis of skin gas that may contain numerous kinds of volatile compounds and compared skin gas with breath.
Di Francesco	Fabio	An analytical procedure for breath sampling has been developed and used in the case of diabetic patients. Bags of different materials have been tested and compared, nalophane guarantees low contamination, maximum stability and limited costs. Clues indicate 2-propanol as a possible marker besides acetone; modifications in breath composition during OGT tests have been studied.
Wagner	S.F.Guenter	¹³ CO ₂ / ¹² CO ₂ -Diagnostic Breath Tests in Gastroenterology, Hepatology, Onkology and Nutrition Control. Organ function, substrate oxidation, metabolic function or dysfunction, bacterial colonisation and overgrowth can be assessed by ¹³ C/ ¹² C isotope ratio at CO ₂ in breath, after administration of a related ¹³ C-substrate. Actual state of the art of ¹³ C-breath testing in its diagnostic applications to be reported.
Španěl	Patrik	SIFT-MS. Water in breath analysis; humidity as an internal validation and total body water measurement using deuterium labelling.
O'Hara	M E	A standardised breath sampling method is now required in breath analysis. This presentation will use research from the breath alcohol testing community to gain insight into the human respiratory system and also show how such research can help in the development of a suitable and convenient breath sampling protocol.
Greenham	Leigh K	As portable low-cost breath analysis instruments become more common, the risk of passing infection from one user to the next must be minimised, without incurring excessive cost for the instrument's owner. Bedford has developed a breath sampling tube for its breath CO instruments which addresses this issue, and laboratory results will be presented.

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Workshop 3. Breath markers in physiology (7 contributions) 90 minutes

Name	FirstName	Summary
Risby	Terence H.	Workshop leader. A personal viewpoint will be presented on the important studies that must be performed so that breath analysis will be accepted by the medical community.
Turner	Claire	An understanding of the breath spectrum in healthy people is essential in the use of breath analysis in the non-invasive diagnosis of disease. This contribution will present findings from a 6 month longitudinal study of 30 healthy volunteers and indicate the factors affecting the breath spectrum.
Davies	Simon J	Experience in breath analysis in both normal subjects and patients with kidney disease.
Bloor	Roger	Overview of the process of clinical development validation of biomarkers in medical research
Sawano	Makoto	CS2 and acetone production after a dose of disulfiram (Anatabuse).
		We developed non-invasive, continuous, high-resolution technique of measuring carboxyhaemoglobin fraction by breath analysis. By application of the technique to carboxyhaemoglobin dilution, we achieved equivalently accurate red cell volume and blood volume measurement with on-fifth infusion volume of CO-saturated blood, and cardiac output measurement without central venous or pulmonary artery catheterization.
Shimouchi	Akito	Chemical compounds in breath originate mainly from volatile metabolic products in health and diseases. Because matrix analysis based on simultaneous measurements of exhaled chemicals with such low mass numbers may give us important information of physical conditions, we conducted the following experiment.
Wang	Tianshu (TS)	Application of breath markers in physiological investigations - A case study on ethanol/D2O ingestion experiment.

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Workshop 6. Confounding variables in breath analysis (5 contributions) 90 minutes

Name	FirstName	Summary
Turner	Claire	Workshop leader. An understanding of the breath spectrum in healthy people is essential in the use of breath analysis in the non-invasive diagnosis of disease. This contribution will present findings from a 6 month longitudinal study of 30 healthy volunteers and indicate the factors affecting the breath spectrum.
Smith	David	The generation of ammonia (from urea) and ethanol (from sucrose) in the mouth and the potential significance to breath analysis will be described.
Ueda	Hideo	Development of oral ammonia (NH ₃) analysis system and application to oral care medicine in practice. We developed an entirely new method (PAT.) to evaluate anaerobes activity in oral cavity. After 20ml of 1% aqueous urea solution is rinsed in oral cavity, and waiting for five minutes with mouth closed, NH ₃ is formed. NH ₃ (10-150ppm) is measured with NH ₃ detector tube, of which color is changed, proportional to NH ₃ amount in length. This system is useful to evaluate of periodontosis, oral malodor, or oral hygiene treatment.
Gov	Yael	Data from Mel Rosenberg's group on mouth odour related research.
Ratcliffe	Norman M.	VOC Metabolites from Stool Samples and Their Influence on Breath VOCs. There are reportably 300-over 3000 VOCs in breath. Many of these compounds have not been fully characterised, nor has the origins of many of these compounds been ascertained. We report the analyses of a wide range of volatile metabolites found in the headspace of stool samples. Over a 100 analyses have now been undertaken from healthy volunteers. The influence of these compounds on breath will be discussed.

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Workshop 4. Clinical breath analysis and lung function (7 contributions) 90 minutes

Name	FirstName	Summary
Schubert	Jochen K.	Workshop leader
Dweik	Raed	Low Levels of Exhaled Nitric Oxide in Severe Asthma. High levels of exhaled nitric oxide (NO) are well documented in mild to moderate asthma but there is currently limited information regarding exhaled NO in severe asthma. We measured NO levels in 36 individual with severe asthma and 82 mild-moderate asthma. Exhaled NO levels showed a significant positive correlation with blood IgE and eosinophils ($p < 0.001$). NO levels in mild to moderate asthma were higher than normal controls. In severe asthma, however, NO levels were lower than mild to moderate asthma and not significantly different from normal controls suggesting unique oxidative abnormalities in the airway milieu of severe asthma.
Basanta	Maria	An adaptive sampler for use with subjects with impaired respiratory function has been developed and it has been used to selectively sample different parts of the breathing profile in COPD subjects over a period of 10 to 15 minutes. GC-MS and GC-differential mobility spectrometry approaches are described.
Modak	Anil S	Arterial paCO_2 is commonly evaluated by an invasive test, the arterial blood gas analysis. The ^{13}C -sodium bicarbonate breath test (SBT) to estimate arterial paCO_2 and clinically significant hypercapnia in patients with obstructive lung disease will be discussed. Percentage of $^{13}\text{CO}_2$ recovered in exhaled breath at 30 minutes (PDR30) alone was able to discriminate hypercapnia ($>45\text{mmHg}$) with a sensitivity of 91% and specificity of 78% ($p < 0.001$).
Roller	Chad	The use of laser spectrometers in clinical studies of exhaled biomarkers. Issues pertaining to calibration, precision, and accuracy over time will be discussed. Results from a 1-year field study measuring NO in diverse populations will be given along with a performance assessment and future work.
Nilsson	Kristofer F	Exhaled NO and experimental pulmonary embolism Increase in exhaled NO in experimental pulmonary embolism. Experimental embolism with either air infusion or homogenates of skeletal muscle tissue was shown to increase exhaled NO in anesthetized rabbits. Inhibition of endogenous NO increased mortality. Exhaled NO should be investigated as an early marker of acute pulmonary embolism. Endogenous NO is protective during embolization.
Cristescu	Simona	Diagnosis of COPD/lung cancer based on exhaled VOCs look very promising: high sensitivity and specificity rates are reported so far in small case-control situations. Unfortunately, these studies do not reflect the actual situation and the population based studies are very much needed. We present here preliminary results obtained within a multi-center lung cancer screening trial. The aim was to detect the prevalence of emphysema and/or lung cancer in (recently quitted) heavy smokers and to determine the diagnostic capabilities of exhaled VOCs.

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Workshop 5. Metabolic disorders (8 contributions) 90 minutes

Name	FirstName	Summary
Fuchs	Dietmar	Workshop leader. Immune response as a source of volatile compounds. Increased neopterin production and accelerated tryptophan degradation predict poor prognosis in cancer patients. Underlying biochemical pathways, GTP-cyclohydrolase and indoleamine (2,3)-dioxygenase, are induced during immune response, and 1-carbon units are set free. Consequently, immune response could underlie the increased formation of compounds like formaldehyde or formic acid in malignancy.
Bloor	Roger	Report of preliminary work on the influence of gastrointestinal motility on breath gases. This presentation will present results of measurement of breath hydrogen levels before and after bowel motions and the role of the faecal mass in production of breath volatiles.
Smith	David	The detection of methanol, ethanol and propanol in breath will be described and the (gut) origin of these alcohols will be tentatively discussed.
Modak	Anil S	5-Fluorouracil (5-FU)/Xeloda are widely prescribed in oncology practice to treat gastrointestinal malignancies. However, 34% of colorectal cancer patients are known to develop severe 5-FU dose-related toxicities. One well-recognized determinant for these observed differences in 5-FU toxicity is the marked (6-fold) variability in the activity of the dihydropyrimidine dehydrogenase enzyme (DPD). The rapid evaluation of DPD enzyme activity prior to 5-FU/Xeloda therapy to minimize potentially life threatening toxicity by the uracil-2-13C breath test will be discussed.
Wagner	S.F.Guenter	13CO ₂ /12CO ₂ -Diagnostic Breath Tests in Gastroenterology, Hepatology, Onkology and Nutrition Control. Organ function, substrate oxidation, metabolic function or dysfunction, bacterial colonisation and overgrowth can be assessed by 13C/12C isotope ratio at CO ₂ in breath, after administration of a related 13C-substrate. Actual state of the art of 13C-breath testing in its diagnostic applications to be reported.
Davies	Simon J	Experience in bringing breath testing from idea to the bedside in a busy clinical environment - what are the pitfalls as well as the benefits. Design of appropriate proof of principle studies. Metabolic disorders of interest include renal failure, diabetes and cardiovascular risk.
Ross	Brian M.	Breath hydrocarbon levels in disorders of the central nervous system. Breath samples were collected from patients with schizophrenia, bipolar disorder, attention deficit hyperactivity disorder and Huntington's disease. Alkane levels were then measured using thermal desorption GCMS. Results from each of these disorders will be presented.
Kushch	Ieugeniia	TCNQ derivatives sensors for diagnostic of upper gastrointestinal disorders. We studied morphological state of gastric mucosa and TCNQ derivatives sensors response to breath gas of 20 adolescents with chronic gastroduodenal pathology and compared obtained data with sensor response of 20 healthy coevals. The results testify that the sensors under investigations are of much interest as a new diagnostic tool.
Khalid	Tanzeela Y.K	Breath analysis for the early recognition of hepatic encephalopathy. Hepatic encephalopathy (HE) is a neuropsychiatric syndrome observed in patients with liver failure and/or portal-systemic shunting of blood. There is not a single, reliable, quick test available for HE detection. Therefore my aim is to identify biomarkers from the breath of patients with HE who often have a characteristic unpleasant breath odour. This could lead the way to a non-invasive, point of care methodology for disease diagnosis. We intend to present a poster discussing our method development and preliminary results

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Workshop 7. *In-vitro* and urine studies (6 contributions) 90 minutes

Name	FirstName	Summary
Smith	David.	Workshop leader. Formaldehyde emitted by urine from cancer patients, and HCN from cultures of <i>Pseudomonas</i> bacterium will be reported.
Fuchs	Dietmar	Immune response as a source of volatile compounds. Weiss M, Ledochowski M, Amann A, Fuchs D, Innsbruck Medical University. Increased neopterin production and accelerated tryptophan degradation predict poor prognosis in cancer patients. Underlying biochemical pathways, GTP-cyclohydrolase and indoleamine (2,3)-dioxygenase, are induced during immune response, and 1-carbon units are set free. Consequently, immune response could underlie the increased formation of compounds like formaldehyde or formic acid in malignancy.
Davies	Simon J	Urine is a rich source of potential biomarkers for disease. I would certainly hope to contribute to this session - mostly from the floor rather than giving a presentation.
Sule-Suso	Josep	Metabolic disorders and cancer. Application of Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) to study the breath of patients with lung cancer and control cases without lung cancer. Also, to study the effects of chemotherapy and/or radiotherapy and correlate breath analysis with treatment response. /// In vitro and urine studies. Application of Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) to study volatiles released by in vitro growing lung cancer cells and to correlate their levels in the headspace with cell number.
Syhre	Mona	Direct diagnosis of <i>Aspergillus fumigatus</i> infection from breath samples. The aim of this study was to identify a unique biomarker of <i>A.fumigatus</i> in the headspace gas of in vitro cultures and to detect the marker from breath samples of infected or colonised patients.
Smith	Stephen	A pilot study of prostate cancer diagnoses by VOC headspace analyses of urine. Prostate cancer was the fourth most common cancer amongst males in England and Wales in 2000. Current detection methods are invasive and expensive. We report the SPME analysis of VOCs from a control group of healthy males and diagnosed patients. This research could lead to a rapid non-invasive detection method.

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Workshop 8. *Panel discussion* (90 minutes)

Panel Discussion will take the form of an open discussion led by the workshop leaders with Patrik Spänel in the chair. The intention is that each of the workshop leaders will be prepared to comment on issues that require further comments and be ready to answer questions from the delegates on topics which they feel have not been adequately dealt with during the workshops.

Specific issues will also be discussed:

- Establishment of a database of volatile compounds in breath (Norman M. Ratcliffe)
- Promotion of the International Association of Breath Research (IABR)
- Venue and organisation of the next meeting
- Presentation of the best poster(s) award(s)

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Other issues that delegates wish to be discussed should be communicated to Patrik Spänel prior to the Panel Discussion.

Poster Sessions. (30)

Name	FirstName	poster	PosterSummary
Barta	Imre	Comparison of Physical and Biochemical Variables of Exhaled Breath Condensate Samples	EBC is a simple and non-invasive technique to collect samples from patients with diseases of the respiratory tract. The reliability of data using such samples is questionable. We aimed to assess the contribution of the choice of condensing equipment to data variability. Volume, conductivity, pH, protein and adenosine was determined from samples obtained with 3 condensers. Measured values scattered for all variables and did not correlate with each other. For most variables, samples from the EcoScreen gave higher readings. We conclude that the type of condenser influences EBC biomarker levels but this alone does not explain the great variability. Chemometric methods allow exploitation of multi-dimensional data for diagnosis and subject monitoring. Sampling is arguably the most important element of the experimental systems used for such studies. Important design factors in breath sampling for metabolomic research are exogenous VOCs, reproducibility, characterisation of artefacts, and the well-being of the subjects. All these factors are addressed in a new adaptive sampler that uses high-purity air supplied to a face mask fitted with pressure transducers for controlling the sampling. Five evaluation experiments are presented: breathing profiles during extended sampling, stability of exogenous VOC profiles, reproducibility of VOC recovery, and breath-profile differentiation.
Basanta	Maria	Adaptive sampling for GC-MS and GC-DMS systems for COPD profiling	Chrometric methods allow exploitation of multi-dimensional data for diagnosis and subject monitoring. Sampling is arguably the most important element of the experimental systems used for such studies. Important design factors in breath sampling for metabolomic research are exogenous VOCs, reproducibility, characterisation of artefacts, and the well-being of the subjects. All these factors are addressed in a new adaptive sampler that uses high-purity air supplied to a face mask fitted with pressure transducers for controlling the sampling. Five evaluation experiments are presented: breathing profiles during extended sampling, stability of exogenous VOC profiles, reproducibility of VOC recovery, and breath-profile differentiation.
Baumbach	Jörg Ingo	Statistical Approaches for Rapid Classification of Lung Diseases by Ion Mobility Spectrometry using Biomarker Data Analysis. J.I. Baumbach, S. Bader, W. Urfer, V. Ruzsanyi, M. Westhoff, P. Litterst, L. Freitag	Volatile Metabolites occurring in human exhaled air are correlated directly to different kinds of diseases. Ion mobility spectrometer (IMS) coupled to multi-capillary columns (MCC) are used to characterize and quantify volatile metabolites occurring in human exhaled breath down to the ng/L- and pg/L-range of analytes within less than 500 s and without any pre-concentration.
Baumbach	Jörg Ingo	Bacterial differentiation by ion mobility spectrometry. - First results of a pilot study P. Litterst, M. Westhoff, L. Freitag, V. Ruzsanyi, J.I. Baumbach	Early diagnosis and specification of bacterial airway infection is of importance, especially in patients who are at high risk for respiratory failure, invasive or non-invasive ventilation and a prolonged hospital stay. Ion mobility spectrometer (IMS) coupled to a multi-capillary-column (MCC) identifies and quantifies volatile metabolites down to the ng/L- and pg/L-range of analytes within less than 500 s and without any pre-concentration. The IMS investigations are based on different drift times of swarms of ions of metabolites formed directly in air at ambient pressure. Head space over selected microbiological cultures was directly sampled for IMS-chromatograms.
Baumbach	Jörg Ingo	Ion mobility spectrometry – a new method for the detection of lung cancer and airway infection in exhaled air? - First results of a pilot study. M. Westhoff, P. Litterst, L. Freitag, V. Ruzsanyi, S. Bader, W. Urfer, J.I. Baumbach	Lung cancer and airway infections gain increasing importance. Early diagnosis is desirable. We examined if volatile metabolites occurring in human exhaled air can be correlated directly to different kinds of diseases. An ion mobility spectrometer (IMS) coupled to a multi-capillary-column (MCC) was used to identify and quantify volatile metabolites occurring in human breath down to the ng/L- and pg/L-range of analytes within less than 500 s and without any pre-concentration. The IMS investigations are based on different drift times of swarms of ions of metabolites formed directly in air at ambient pressure.
Beauchamp	Jonathan	PTR-MS Applications in Life Science	Proton Transfer Reaction-Mass Spectrometry (PTR-MS) is an analytical technique for detection and quantification of volatile organic compounds (VOCs) in air. The very sensitive PTR-MS instrument is capable of detecting VOCs on-line (within seconds) and at very low concentrations (detection limit in the pptv range), and requires no sample preparation before analysis. This makes it an ideal tool for analysis of breath, or urine/blood headspace, in order to detect potential VOC markers for certain diseases. A general overview of PTR-MS and its applications in the life sciences will be presented.
Cordell	Rebecca L	Detection of Chemical Warfare Simulants and Hydrolysis products using Chemical Ionisation Time-of-Flight Mass Spectrometry.	One of the critical requirements in dealing with chemical attacks is the need for rapid and accurate triage. To combat this, a real-time screening technology based on breath analysis is being developed, potentially allowing medical assessment of victim status following a chemical attack to identify the causative agent and the exposure level. Using a CIR-TOF-MS method various hydrolysis products and simulants of G- agents and sulphur mustard have been successfully characterised showing the potential for application of CIR-TOF-MS to detection of chemical agents in breath.
Cristescu	Simona	Detection of emphysema from unselected smoker via exhaled volatile organic compounds	Diagnosis of COPD/lung cancer based on exhaled VOCs look very promising: high sensitivity and specificity rates are reported so far in small case-control situations. Unfortunately, these studies do not reflect the actual situation and the population based studies are very much needed. We present here preliminary results obtained within a multi-center lung cancer screening trial. The aim was to detect the prevalence of emphysema and/or lung cancer in (recently quitted) heavy smokers and to determine the diagnostic capabilities of

			exhaled VOCs.
Davies	Simon J	Deuterium kinetics in haemodialysis patients and the optimal time schedule for breath sampling in determination of total body water (TBW) using Flowing Afterglow Mass Spectrometry (FAMS)	This poster will describe how we have developed a breath test to enable measurement of body water in the clinical environment. It will demonstrate how we have optimised our sampling strategy by gaining a full understanding of deuterium kinetics in haemodialysis patients. By the time of the conference we will have commenced our first proof of principle study, so we hope to include early data from this.
Fritsch	Thomas	Laserspectroscopic Online Analysis of Exhaled Carbon Monoxide	We report online measurements of exhaled carbon monoxide using infrared cavity leak-out spectroscopy (CALOS). One of the advantages of the CALOS approach is the ability of detecting different isotopologues of one molecule at the same time, e.g. ^{12}CO and ^{13}CO . One application of this special benefit could be using ^{13}CO as a tracer molecule for physiological studies. We present the spectrometer used and our latest results on isotopologue-selective measurements of CO in human breath.
Fuchs	Patricia	Breath aldehydes as markers of disease	Oxygenated compounds such as aldehydes and ketones in breath have been linked to metabolism, oxidative stress and cancer. Concentrations of aldehydes in breath were assessed quantitatively by means of solid phase micro extraction, on fiber derivatization (SPME-OFD) and GC/MS. Mechanically ventilated patients with various diagnoses and healthy volunteers were studied. C2 – C7-aldehydes were determined simultaneously with a LOD of 10 - 50 nmol/l. In a pilot study differences of aldehyde concentrations could be seen between healthy volunteers and critically ill patients. This new analytical technique bears the potential of non invasive diagnostic and therapeutic monitoring.
Garner	Katy E	Volatiles in NEC a Novel detection method	Necrotizing Enterocolitis. This is a serious gastrointestinal disease affecting predominantly premature babies. The incidence of NEC is 1%-5% of all NICU admissions with a high mortality of 20-40%. Early diagnosis is difficult due to the non specific nature of the symptoms. It has been noted that a preterm infant is likely to have a more similar bacterial gut colonisation due to the hospital environment compared to a term infant; therefore by analysing the volatile organic compounds from the faeces; using headspace SPME, in these infants a biomarker may become evident. Three centres; Bristol and two in Birmingham have agreed to take part in this study.
Greenham	Leigh K	Infection control techniques for portable low-cost breath gas analysers	As portable low-cost breath analysis instruments become more common, the risk of passing infection from one user to the next must be minimised, without incurring excessive cost for the instrument's owner. Bedford has developed a breath sampling tube for its breath CO instruments which addresses this issue, and laboratory results will be presented.
Ipei	Takahashi	Expiratory carbon monoxide in a Japanese population + Relationship between expiratory carbon monoxide and neutrophil-related reactive oxygen species in a Japanese population	Endogenous carbon monoxide (CO) is known to impart protection against oxidative stress. However, few epidemiological studies have surveyed the expiratory CO concentrations in the general population. In this study, the expiratory CO concentrations were measured with a CO analyzer in 276 males and 606 females. The subjects were residents of Iwaki town, Aomori Prefecture in northern Japan, with ages over 20. Expiratory CO concentrations decreased in direct proportion to increasing age, but increased in smokers and alcohol drinkers. + Endogenous carbon monoxide (CO) can protect the human body against oxidative stress, whereas reactive oxygen species (ROS) acts as a stressor. However, no epidemiological studies have surveyed the relationship between expiratory CO concentrations and the ROS production capability of neutrophils in the general population. In this study, the expiratory CO concentrations and ROS production capability were measured in 276 males and 606 females. The subjects were residents of Iwaki town, Aomori Prefecture in northern Japan, with ages over 20. A weak correlation was seen between these two parameters (n=879, r=-0.07, p<0.05 using Spearman's rank correlation).
Khalid	Tanzeela Y.K	Breath analysis for the early recognition of hepatic encephalopathy	Hepatic encephalopathy (HE) is a neuropsychiatric syndrome observed in patients with liver failure and/or portal-systemic shunting of blood. There is not a single, reliable, quick test available for HE detection. Therefore my aim is to identify biomarkers from the breath of patients with HE who often have a characteristic unpleasant breath odour. This could lead the way to a non-invasive, point of care methodology for disease diagnosis. We intend to present a poster discussing our method development and preliminary results
Kischkel	Sabine	Sampling and Sample Stability in Breath Analyses	Steps prior to analysis such as sampling and preconcentration may impact results. In this study different methods of breath sampling were compared in terms of end tidal pCO ₂ and pCO ₂ in the samples. In addition, stability of gaseous samples in bags and glass vials was accessed. Lowest differences between pCO ₂ et and pCO ₂ sample and lowest RSD's were found in alveolar gas samples that had been collected in bags or gas tight syringes. Impact of storage onto concentration of volatile substances in the samples depended on septum/bag materials and physico-chemical properties of the substances.
Mochalski	Pawel	HS/GC methods for Ne and	Currently, the MIGET test is the only reliable method for the determination of a ventilation-perfusion ratio of the lung. However,

		SF6 determination in breath and blood	the method is invasive and requires injection of suitable gases. That's why gases with properties similar to MIGET gases and existing in blood at steady concentrations are sought. Within this work HS/GC (head space/gas chromatography) methods for the determination of Ne and SF6 in breath and blood are presented. Neon is measured with a doped with neon PD-HID detector (pulse discharge helium ionization detector) whereas SF6 with a PDHID detector working in the ECD mode.
Nose	Kazutoshi	Relationships between compositions of volatile chemical compounds in breath and skin gas detected by a high sensitive method	We developed a skin gas sampling system consisted mainly of flow controllers, gas cleaners and a chamber in which purified gas circulated the skin surface. The skin gas was carried and introduced into highly sensitive APIMS and/or gas chromatography. The mass spectrums of skin gas released from the palms were well reproduced in both negative and positive ionization modes. Most of chemicals exhibited significantly linear relationships between the concentrations of skin gas and breath in healthy subjects, while there were several specific chemicals to the skin gas or to breath.
Roller	Chad	Laser Spectroscopic Measurements of Nitric Oxide in Feedyard Cattle	Measurement of nitric oxide (NO) in the expired breath of crossbred calves received at a research facility was performed using tunable diode laser absorption spectroscopy (TDLAS). A custom breath collection system was designed to collect lower airway breath of spontaneously breathing calves while in a restraint chute. Breath was collected and analyzed from calves upon arrival and periodically during a 42-day receiving period. There was a statistically significant relationship between eNO, severity of bovine respiratory disease (BRD) in terms of number of times treated, and average daily weight gain over the first 15-days post arrival.
Shimouchi	Akito	Factors affecting expired minute volumes of low-molecular weight compounds	Fasted 960 volunteers aged from 20 to 88 years old breathed purified artificial air via a mouthpiece in a sitting position for 12 min, during which exhaled air was collected via one-way valve into the Douglas bag. Minute ventilation volume and concentrations of CO ₂ and O ₂ in exhaled air were monitored. Concentrations of H ₂ , CH ₄ , CO, NO and NO ₂ (= Nox - NO) in the bag were also analyzed. We will present the relationships between minute expired volumes of these compounds and such physical conditions as age, gender, laboratory data, scores of health-related questionnaires, and diseases.
Španěl	Patrik	Combined use of gas chromatography and selected ion flow tube mass spectrometry for absolute trace gas quantification	The value of the gas chromatography (GC) and selected ion flow tube mass spectrometry (SIFT-MS) combination for the analysis of trace gases is demonstrated by the quantification of acetone in air samples using the three precursor ions available to SIFT-MS, viz. H ₃ O ⁺ , NO ⁺ and O ₂ ⁺ , and by the separation of the isomers 1-propanol and 2-propanol, and their analysis using H ₃ O ⁺ precursor ions. It is shown that the GC/SIFT-MS combination allows for accurate trace gas quantification obviating the regular, time-consuming calibrations that are usually required for the more commonly used detectors of GC systems, and the positive identification of isomers in mixtures that is often challenging using SIFT-MS alone.
Thelen	Sven	Laserspectroscopic Online Monitoring of Ethane Traces in Exhaled Breath	Major breath analyzer development activities are directed towards mobile devices with sub-ppb sensitivities. Here we report on advances in extremely sensitive and specific online analysis of trace gases by means of a transportable mid-infrared laser spectrometer. We are evaluating in particular Cavity Leak-Out Spectroscopy (CALOS) for the quantitative online detection of ethane which is considered as the most important volatile marker of free-radical induced lipid peroxidation. We currently achieve an ethane detection limit of 400 ppt or 0.4 n/l and a time resolution of better than 0.8 s which is sufficient for the time-resolved online measurement of single exhalations.
Thomas	Paul	Dispersion field strength programming in exhaled breath analysis with differential mobility spectrometry	Differential mobility spectrometry exploits the declustering phenomena of molecular ions when subjected to 10 to 30 kV/cm ⁻¹ electric field strengths at atmospheric pressure. The combination of DMS with thermal desorption GC provides a new and potentially powerful technique for the trace analysis of breath in the clinic or out in the field. An exciting development is the use of programmable dispersion fields within DMS in conjunction with temperature programming to expand the analytical space of the approach. The use of thermal desorption GC-DMS with programmable dispersion fields in the profiling of asthmatic subjects is described and preliminary data presented.
Turner	Claire	Concentration Distributions of common Breath Metabolites in the healthy Population	The concentration distributions of ammonia, acetone, isoprene, methanol, ethanol, propanol and acetaldehyde were determined using on-line SIFT-MS analyses of breath of 30 healthy volunteers over a 6 months period.
Ueda	Hideo	The smallest hydrogen (H ₂) analyzer and clinical application + A new flatus monitor and the significance in practical medicine	We developed a compact, and easy-to-operate hydrogen (H ₂) analyzer for clinical practice to measure breath and oral gas, separately. H ₂ in breath and oral gas is the product of anaerobes living in our body; breath H ₂ is a indicator of intestinal, and oral H ₂ is of oral bacterial movement. Previously, H ₂ is used for a kind of diagnosis of digestive organs. Recently, it is known that "active hydrogen" shows SOD-like activity in biological study. Simple and rapid H ₂ determination is needed at bedside situation. To detect H ₂ , a sensitive and specific hydrogen gas sensor, which is housed in sensor probe to detect H ₂ with rapid and reliable response, and the

			<p>result is printed. We expect the clinical application of H₂ Analyzer to diagnosis of intestine movement, an effective marker after dosage of hepatic drugs, for example, and oral care index, respectively. Detecting the passage of flatus is important in the diagnosis of gastrointestinal movement, especially, when treating post operative patients because it shows recovery of bowel function. Since hydrogen (H₂), like CO₂, is always in flatus, H₂ can also be used as an indicator of flatus. The amount of H₂ in expired air is far less than for CO₂ and may not affect deflections from the H₂ baseline. And because the H₂ detector is more sensitive and accurate, besides a small-size than the CO₂, it is preferred to a CO₂ analyzer for detecting flatus. As a flatus monitor, we developed a compact and simple bedside-use H₂ detector system, and compared this H₂ detecting with CO₂. Tracings of the H₂ baseline were more stable than those of CO₂, and a clear peak was recorded after the passage of flatus. Practical use of the flatus monitor in clinical situation will be expected in near future</p>
Vaittinen	Olavi	A high repetition rate cavity ringdown spectrometer	<p>Our presentation describes the construction of a sensitive high repetition rate cavity ringdown spectrometer (CRDS) in the near infrared. The set-up is based on a Ti:sapphire ring laser and a high-finesse Fabry-Perot interferometer. A feedback system using a Pound-Drever-Hall locking scheme has been built to lock the laser frequency to the maximum of a transmission fringe of the interferometer. The main advantage of the system is that the ringdown events can be generated at a rate of 10 kHz which is 100 times faster than in the usual CRDS experiments. Minimum detectable absorptions as small as 2 x 10⁻¹¹ cm⁻¹ have been achieved for standard operating conditions. The latest spectra recorded with the spectrometer will be presented to illustrate its sensitivity and applicability to, for example, breath analysis.</p>
Wagner	S.F.Guenter	13C-Breath Tests to assess Hepatic Function and Disease Severity in Liver Diseases.	<p>The breath test using 75mg 13C-Methacetine as the substrate to check the de-methylation and carboxylation by the microsomal liver function will indicate for a patient any liver damage from former or actually active liver diseases. Diagnostic assessments available from that breath test are Cirrhosis rated Child-Pugh C/B or A, Steatosis/Fibrosis, Normal, Stimulated. Evolution of a "fatty liver" can be followed from a very early stage down to cirrhosis, and a Tumor liver is indicated with its left-over capacity. Non-invasive. and non-radioactive, all the 13C-liver-breath tests form a patient-friendly alternative to the liver-biopsies.</p>
Whyte	Christopher	Hadamard Transform CIR-TOF-MS: A High Sensitivity Instrument For Breath Analysis	<p>The Chemical Ionisation Reaction Time of Flight Mass Spectrometer (CIR-TOF-MS) used in our laboratory has been shown to be a versatile instrument for the detection of trace gas VOC species in breath. The newly developed technique of Hadamard Transform CIR-TOF-MS improves upon conventional TOF-MS by employing a multiplexing procedure that increases the instrument's sensitivity. In coupling high detection sensitivity to the real-time and multi-channel analysis capability of TOF-MS, we have developed an instrument that is a powerful analytical tool for the detection of trace VOC species within human breath.</p>
Willis	Kerry	Breath Analysis using Chemical Ionisation Reaction Time-of-Flight Mass Spectrometry	<p>Chemical Ionisation Reaction Time-of-Flight Mass Spectrometry (CIR-TOF-MS) has been developed to measure trace volatile organic compounds in exhaled breath as a real time, non-invasive tool for medical diagnosis and monitoring. The instrument features a typical detection limit of the order of parts-per-billion in one second and the multichannel detection capability of TOF-MS means simultaneous detection of the broad range of VOCs present in exhaled breath. Initial studies with a basic sampling device have shown a number of VOCs can be detected using both H₃O⁺ and NO⁺ reagent ions.</p>
Yamada	Masuyoshi	Mass analysis of breath VOCs using adsorbent sampling filter	<p>A new breath analyzing system using mass spectrometer has been developed. VOCs in a breath sample are collected on adsorbents in a breath sampling filter and analyzed by gas chromatography (GC) / atmospheric-pressure chemical ionization (APCI) / mass spectrometer (MS). During breath sampling, the subject experiences no resistance because the pressure loss of new breath sampling filter is lower than 1 kPa, while that of the conventional adsorbent tube is 50 kPa. The sensitivity of the total system is sub ppb.</p>

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